

Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage

**Bart A. van Hassel, D. Mosher, J.M. Pasini,
M. Gorbounov, J. Holowczak, S. Hay, J. Khalil,
F. Sun, X. Tang and R. Brown**
United Technologies Research Center



DOE Hydrogen Program

Annual Merit Review

Washington, DC

June 8, 2010



**United Technologies
Research Center**

Project ID: ST006

Overview

■ Timeline

- Start: February 2009
- End Phase 1: July 2011
- End Phase 2: July 2013
- End Phase 3 / Project: July 2014
- Percent complete: 18.0% (spending)

■ Budget

- \$6.86M Total Program
 - \$5.32M DOE
 - \$1.55M (22.5%) UTRC
- FY09: \$350k DOE
- FY10: \$870k DOE

■ Barriers*

- A – J
- A. System Weight & Volume
- E. Charging / Discharging Rates
- J. Thermal Management

■ Targets*

- All

■ HSECoE Partners



* DOE EERE HFCIT Program Multi-year Plan for Storage

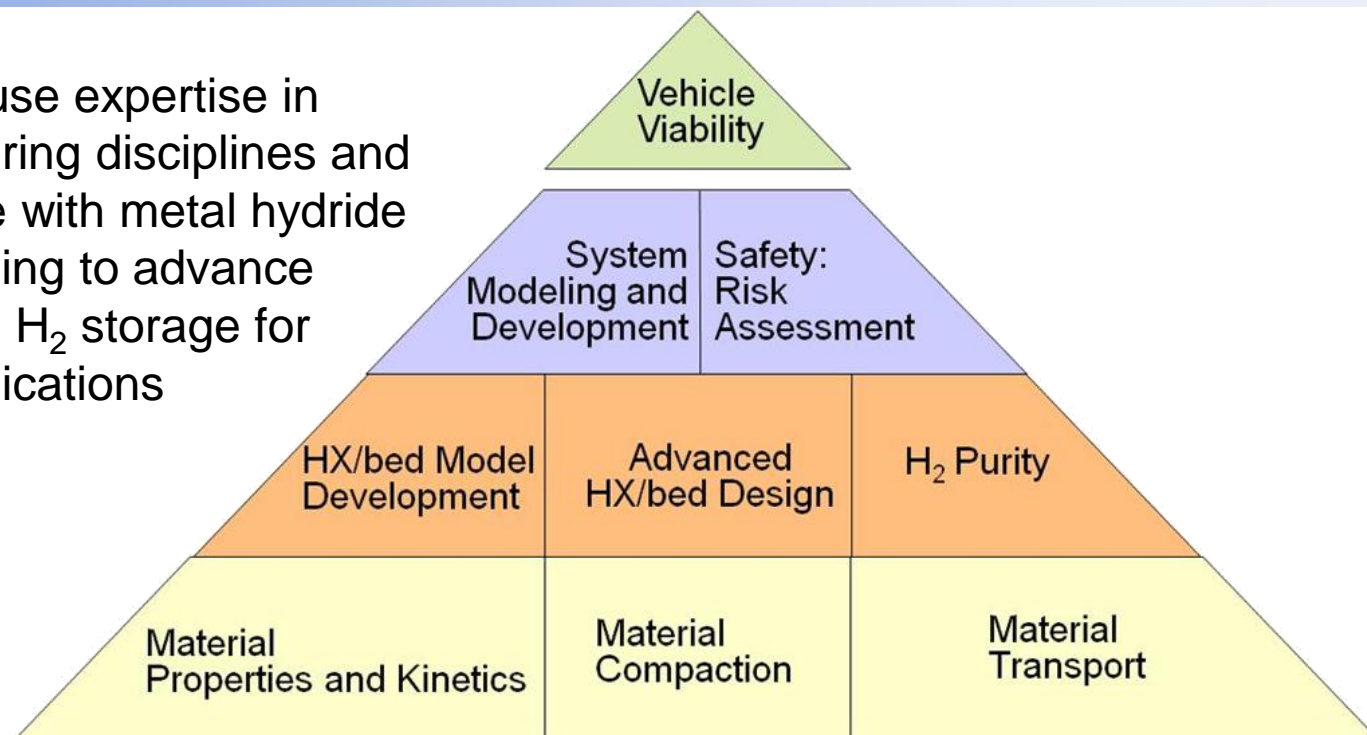
Objectives

- Design of materials based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles
- H₂ storage system focus:
 - Metal hydride
 - Chemical hydride
 - H₂ cryo-sorption materials
- Target examples:

Performance Measure	Units	2010	2015	Ultimate
System Gravimetric Capacity	g H ₂ /kg system	45	55	75
System Volumetric Capacity	g H ₂ /L system	28	40	70
System fill time (for 5 kg H ₂)	minutes	4.2	3.3	2.5
Fuel Purity	% H ₂	SAE J2719 guideline (99.97% dry basis)		

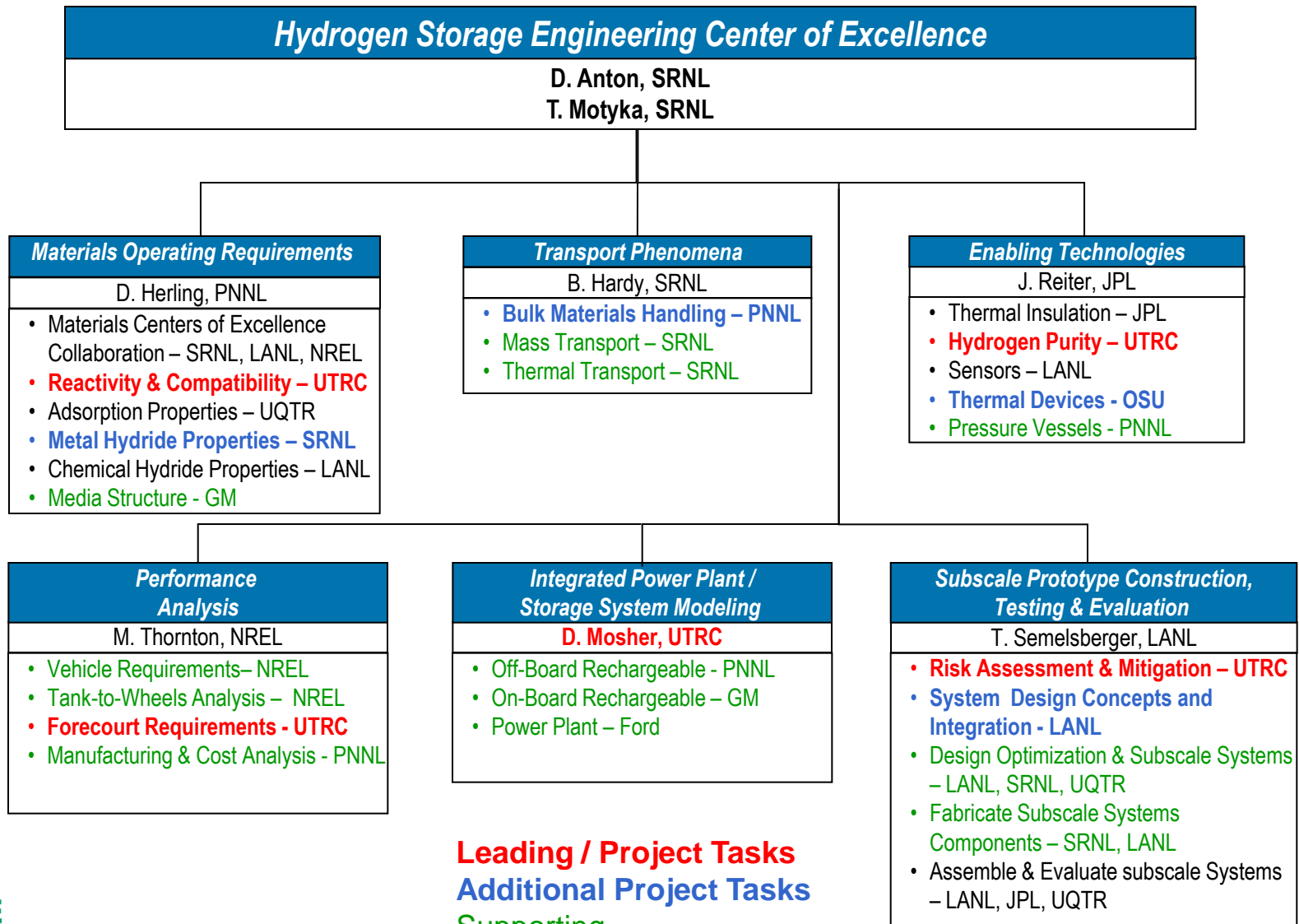
Approach

- Leverage in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials based H₂ storage for automotive applications

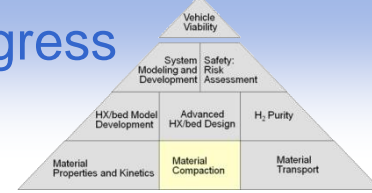


Month/Year	Go/No-Go Decision
Apr-11	Provide a system model for each material sub-class (metal hydrides, adsorption, chemical storage) which shows: <ul style="list-style-type: none"> • 4 of the DOE 2010 system storage targets are fully met • Status of the remaining targets must be at least 40% of the target or higher

Center Structure – Roles & Collaborations



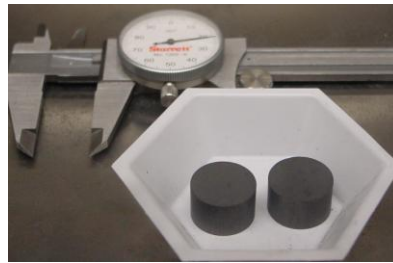
Engineered Compaction



- Objective: Improve volumetric capacity and thermal conductivity through powder compaction
- Coordinated through GM



Press inside glovebox

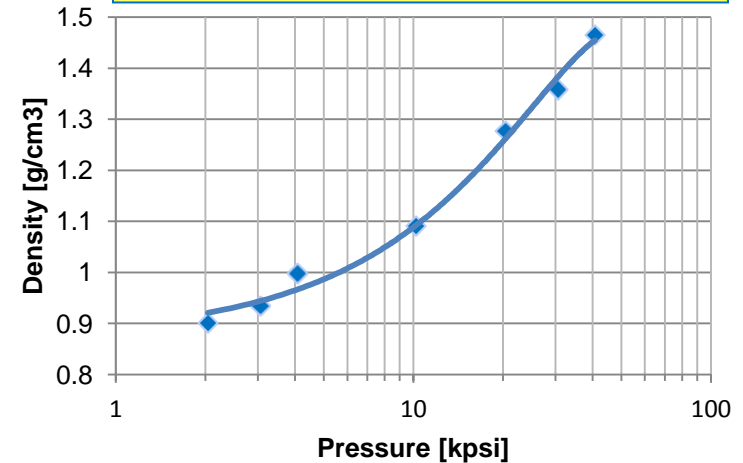


Pellets for thermal Conductivity measurements

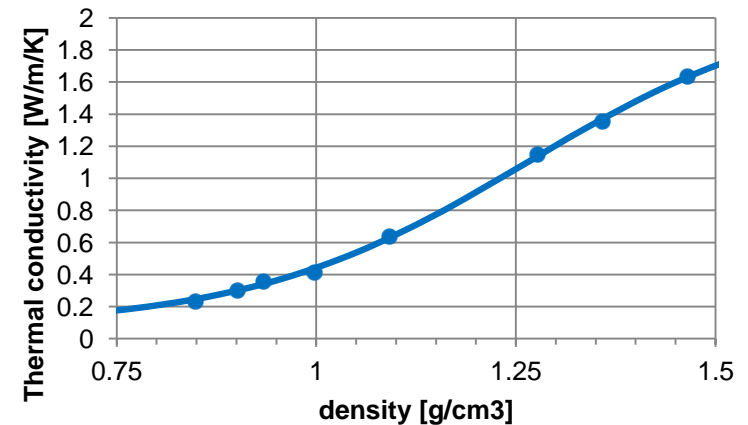


Thermal conductivity analyzer

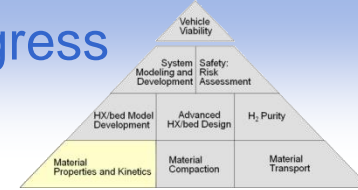
Density increased by 63%
(39% reduction in volume)



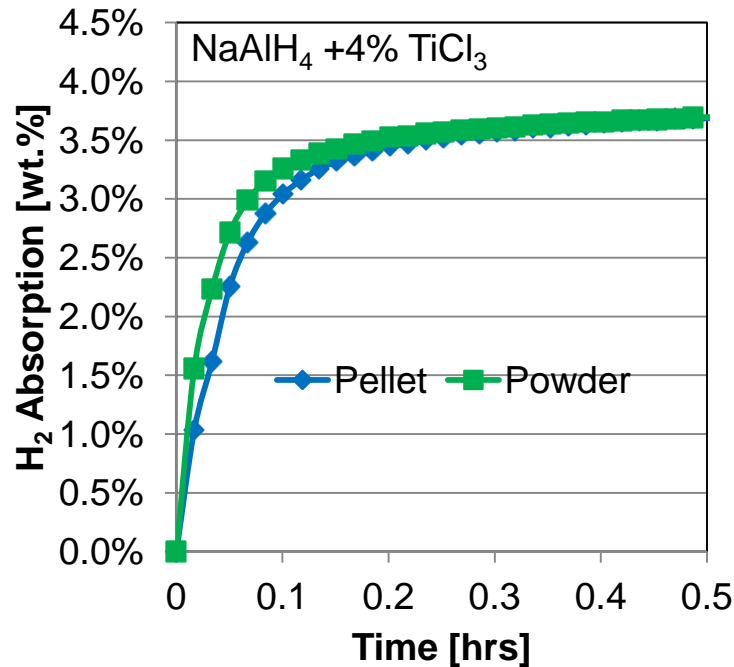
7X improvement of thermal conductivity



Properties of Compacted Metal Hydride

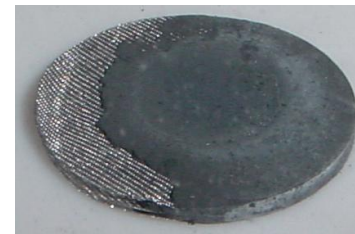
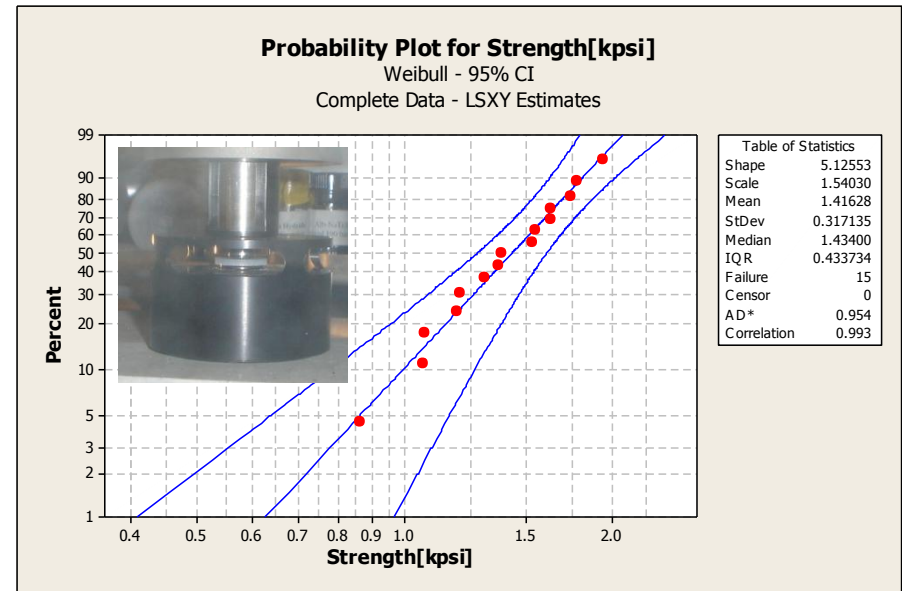


- H₂ Absorption (120°C, 110 bar)



Comparable H₂ absorption and desorption rate before and after compaction

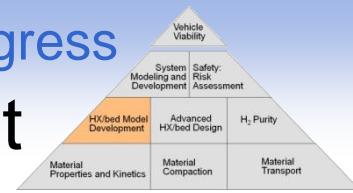
- Biaxial flexure screening test for compressed pellets



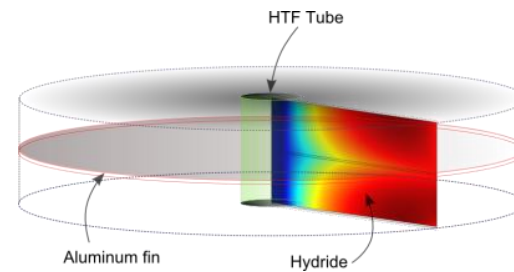
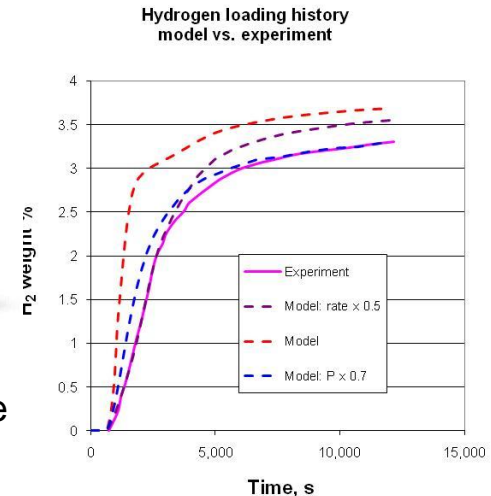
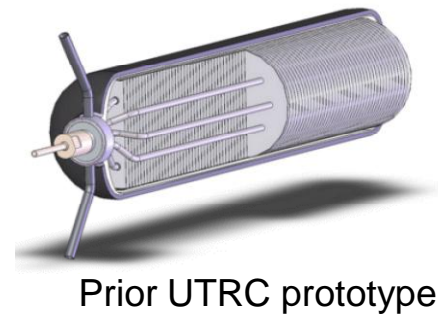
Reinforced NaAlH₄

Integrating pellet reinforcement and thermal conductivity enhancement in compacted material

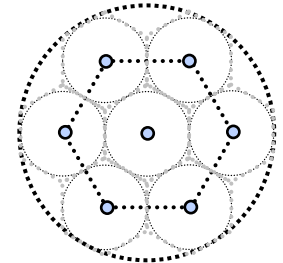
Storage System Model and HX Development



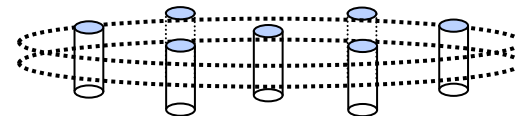
- Objective: Optimization of hydrogen storage system heat exchanger for fast refueling time
- Approach:
 - Co-developed and validated COMSOL™ model of NaAlH₄ bed with SRNL
 - Incorporated improved material properties after compaction (ρ , k)
 - Performed parametric study to optimize heat exchanger design for fast refueling time
 - Developed lumped parameter model for System Level Modeling



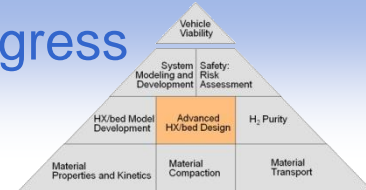
Finite element model



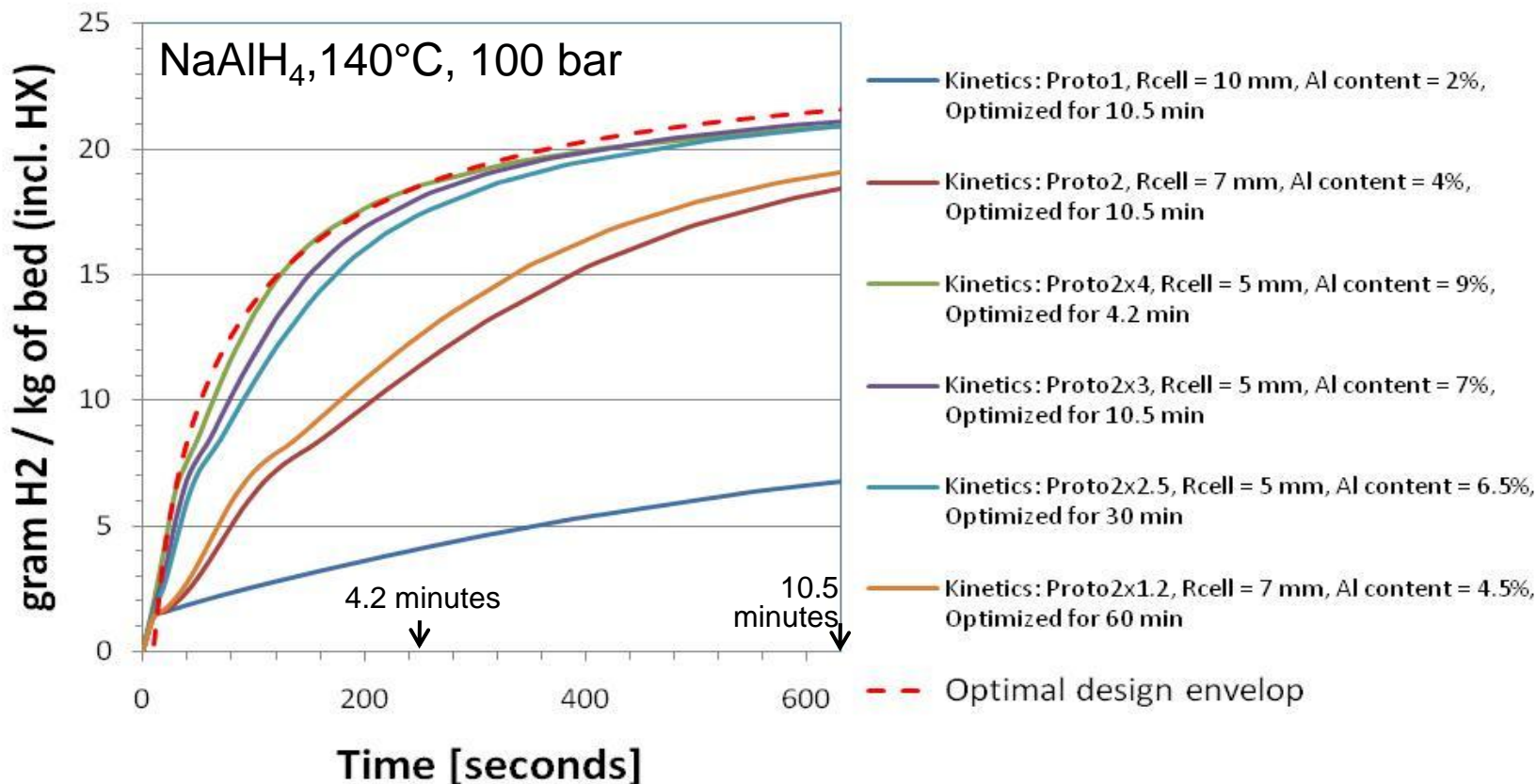
Parametric model



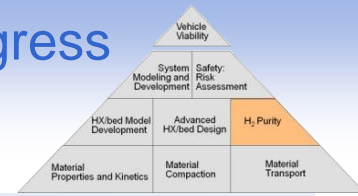
HX Design for Fast Refueling Time



- Different bed designs are optimal for specific refueling times



NaAlH₄ is a good model material for designing engineering tools but can not achieve gravimetric capacity targets at fast refueling times

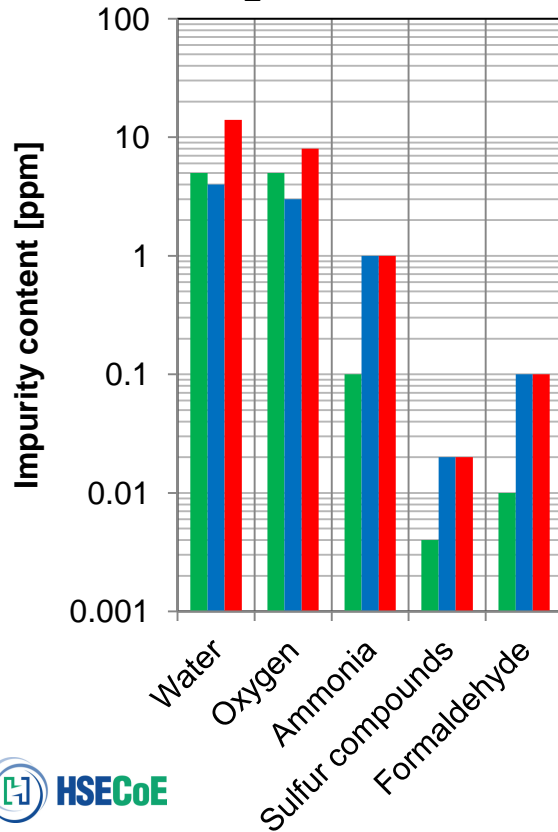


H₂ Purity

- Objective: Develop system methods to improve discharged hydrogen purity / quality for acceptable PEM fuel cell durability

Impurities of Concern:

- NREL H₂ Forecourt



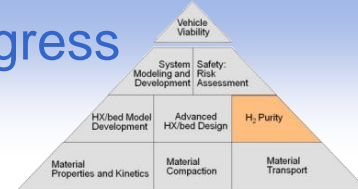
- Based on HSECoE Tier 1 & 2 Materials

Storage material	Impurity	SAE guideline	HSECoE Estimate
Ammonia Borane	Borazine	???	0.4-3.0%*
	Diborane	???	1-5 ppm
	Ammonia	0.1 ppm	20-200 ppm
Metal Amides	Ammonia	0.1 ppm	200-800 ppm

*LANL: 0.01-0.08 mol Borazine/ mole of AB reacted

Initial focus on Ammonia

Preliminary Purification System Comparison

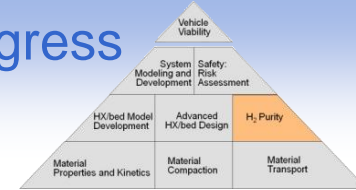


Factor	Conventional Palladium Membrane	Regenerable Physical Adsorption	Chemical Adsorption
Weight	Heavy	Heavy ¹⁾	Light
Volume	Big	Big	Small
Cost	Expensive	Affordable	Affordable
H ₂ loss	2-5%	High¹⁾	Low
Pressure	>50 psig	High pressure preferred	Atmospheric or high pressure
Temperature	300-400°C	RT	RT<T<150°C
Purity	99.99999999%	99.97%	99.97%
Life expectancy	>5 years	>2 years	3 month replacement

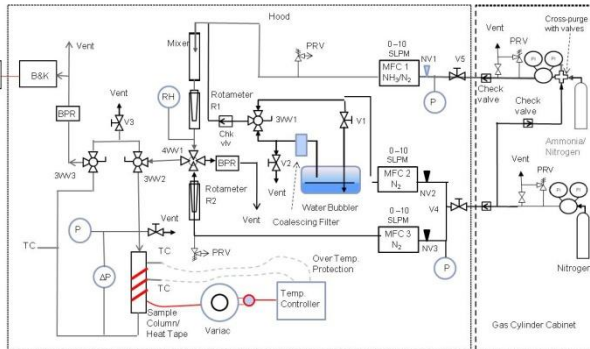
¹⁾ Assuming on-board regeneration

Chemical adsorption cartridge selected for Ammonia

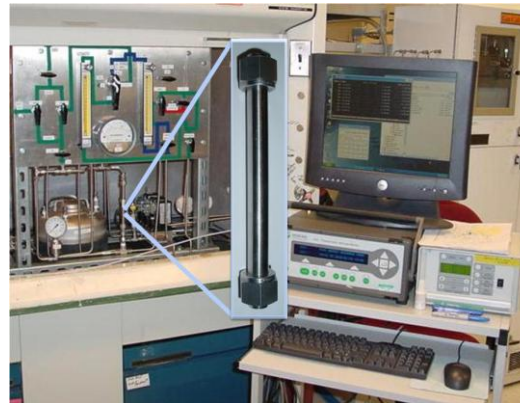
Adsorption System Development



Process Flow Diagram



Test apparatus

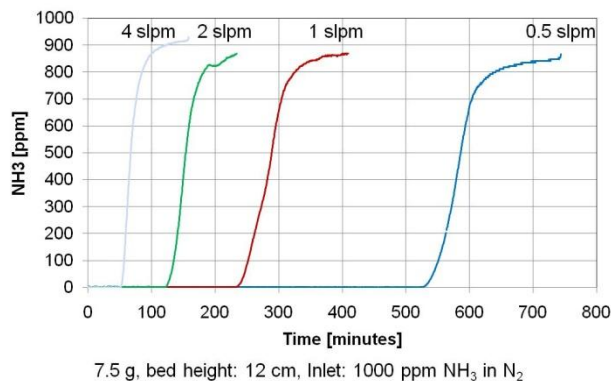


NH₃ adsorbent

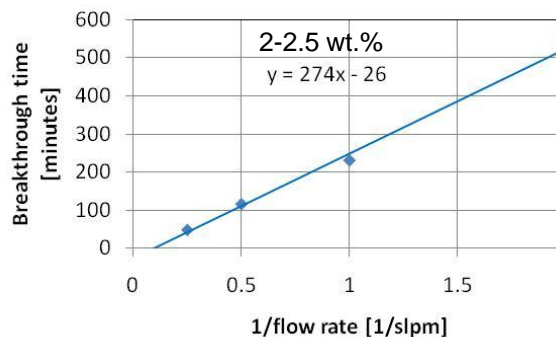
- Mesh size: 20x30 mesh (0.84x0.60 mm)
- Tap Density: 0.673 g/cm³
- BET surface area: 673 m²/g
- Pore volume: 0.338 cm³/g
- Average Pore Diameter (4V/A by BET): 20.1 Å



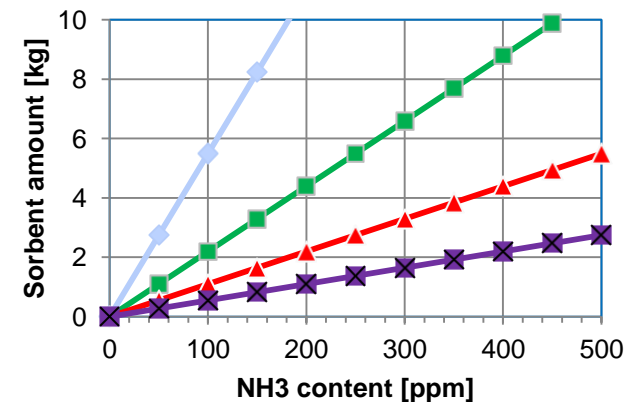
NH₃ breakthrough curves



Flow rate dependence NH₃ breakthrough time

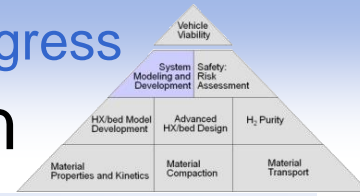


Cartridge weight for 3-month replacement interval

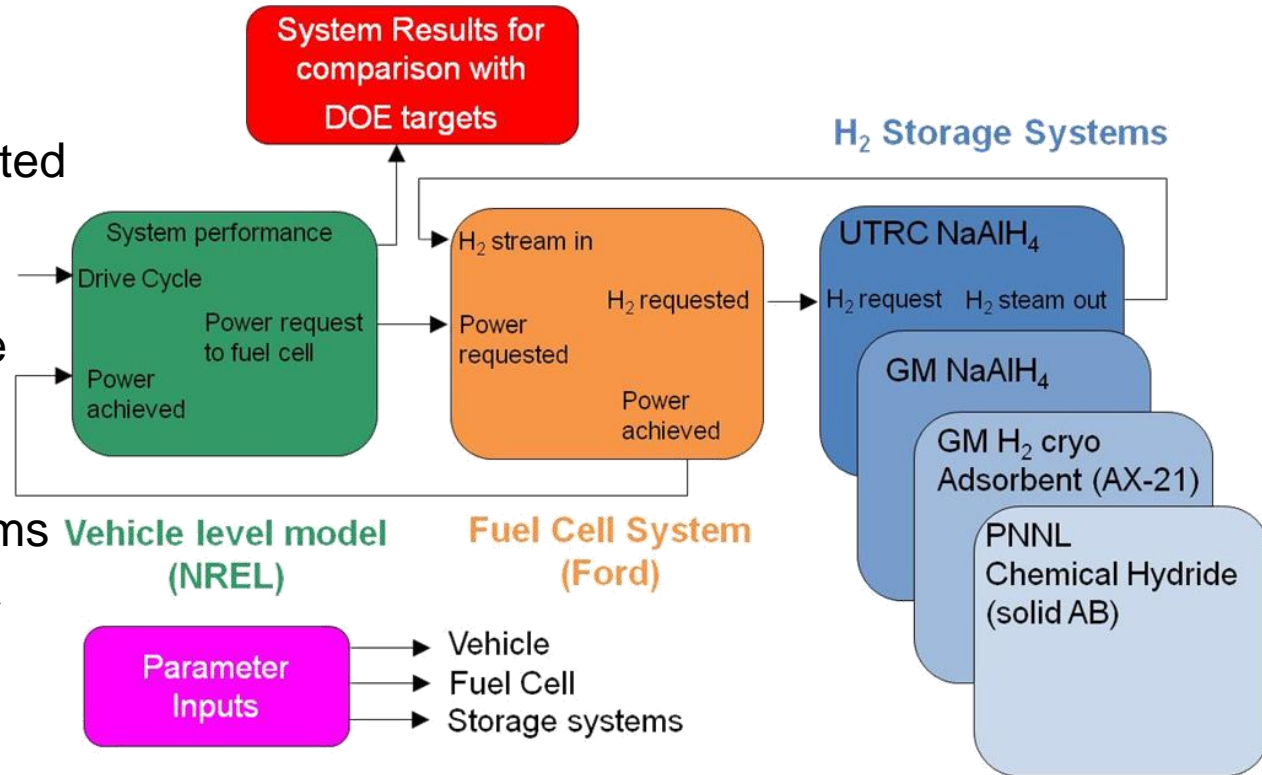


Adsorbent based H₂ purification cartridge for NH₃ appears viable

Integrated Framework for Vehicle Simulation

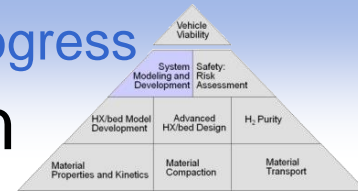


- Objective: Evaluate combined power plant / storage system configurations to determine hydrogen storage system requirements and predict overall performance
- Progress:
 - Framework structure developed and implemented in Simulink™
 - Different storage system types coexist within same framework
 - Results generated for comparing storage systems against DOE targets on a common basis



UTRC leading IPP/SSM technical area and providing support to all partners for implementing their contributions

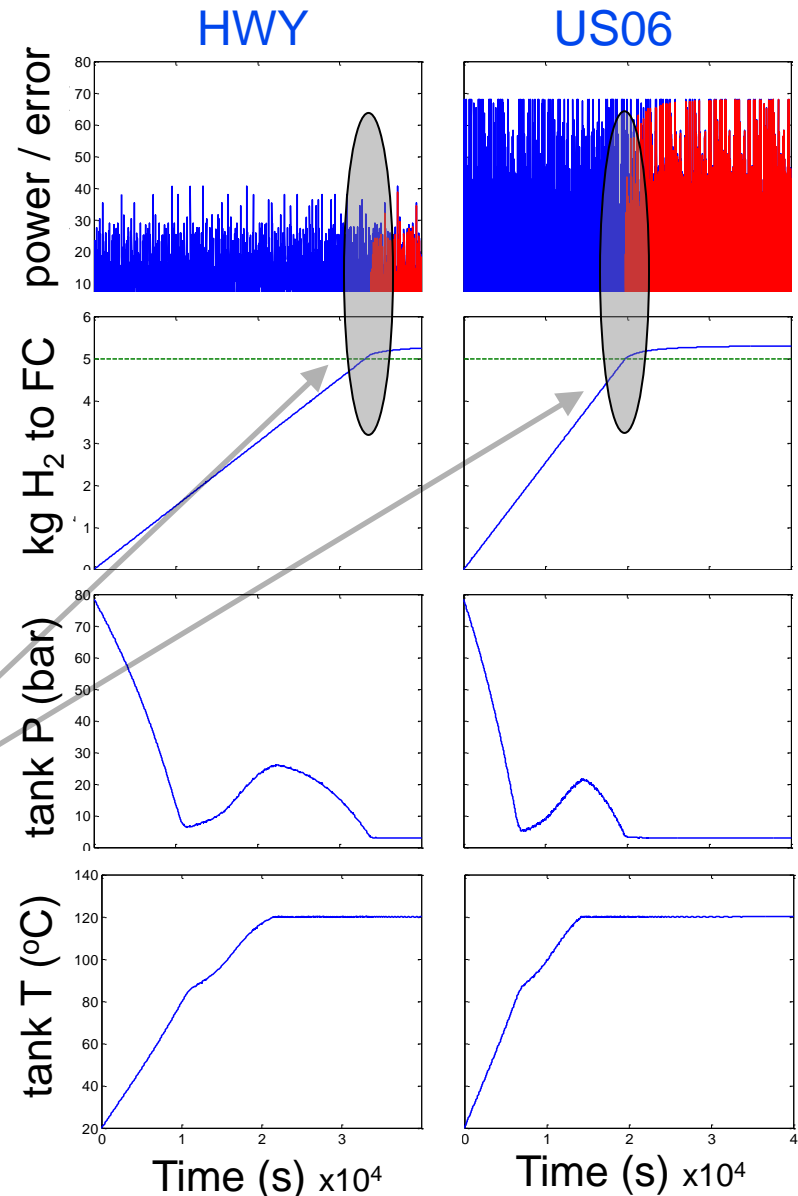
Integrated Framework for Vehicle Simulation



NaAlH₄ system example:

- Power demand curves from HSSIM (NREL)
- Lumped heat transfer model parameters from COMSOL™ model of NaAlH₄ bed
- Single “cold start” from 20°C:
 - H₂ stored in free volume is burned to raise temperature
- Drive cycle repeats indefinitely
 - Drive cycles were not designed for vehicles with materials based H₂ storage systems
- Minimum delivery pressure: $P_{\min} = 3$ bar
- Results show drive cycle is tracked correctly until **after** 5kg H₂ have been delivered to the fuel cell.
- More details in presentation by GM

Performance comparison of all three hydrogen storage systems on a common basis



FY10 and FY11 Plan

	FY10		FY11		
	3Q	4Q	1Q	2Q	3Q
Improve properties through compaction with reinforcing material	■				
Quantify impact of pressure gradients inside consolidated metal hydride powder on H ₂ absorption and desorption kinetics	■				
Evaluate small test article with structured media	■	■			
Evaluate alternative reversible metal hydride materials in common H ₂ storage framework with current engineering tools		■	■	■	
Improve capacity of on-board H ₂ purification cartridge for ammonia	■	■			
Develop and assess methods for removing boron containing species	■	■			
Qualitative risk assessments of novel systems	■	■	■	■	■
Improve definition of Balance of Plant (BOP) components in system model and establish a common bill of materials	■				
Implement initial cost model library for storage systems		■			
Identify technology gaps and prioritize concepts	■				
Quantify hydrogen storage system performance against DOE targets for Go/No-Go decision on April 30, 2011	■	■	■	■	★

Summary

Relevance: Design of materials based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles

Approach: Leverage in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials based H₂ storage for automotive applications

Technical Accomplishments and Progress:

- Developed method that improved volumetric capacity and thermal conductivity through compaction
- NaAlH₄ is a good model materials but can not achieve gravimetric capacity targets at fast refueling times
- Hydrogen purification cartridge for adsorbing NH₃ appears viable
- Established Simulink framework that enables performance comparison of all three hydrogen storage materials against DOE targets on a common basis

Collaboration: Active collaboration with all partners in center, for instance between Ford, GM, PNNL and NREL on system level modeling

Future Work: Work towards milestones on quad charts of each of the technical areas and technical teams and towards Go/No-Go decision on April 30, 2011

Acknowledgements

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